

## Lower bounds on entanglement measures from incomplete information

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How can we quantify the entanglement in a quantum state, if only the expectation value of a single observable is given? This question is of great interest for the analysis of entanglement in experiments, since in many multiparticle experiments the state is not completely known. We present several results concerning this problem by considering the estimation of entanglement measures via Legendre transforms. First, we present a simple algorithm for the estimation of the concurrence and extensions thereof. Second, we derive an analytical approach to estimate the geometric measure of entanglement, if the diagonal elements of the quantum state in a certain basis are known. Finally, we compare our bounds with exact values and other estimation methods for entanglement measures.

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### I. INTRODUCTION

Entanglement is a key phenomenon in quantum-information science and the quantification of entanglement is one of the major problems in the field. For this quantification many entanglement measures have been proposed [1–9]. However, a central problem in most of these proposals is the actual calculation of a given measure: entanglement measures are typically defined via optimization procedures, which may consist of a maximization over certain protocols or the minimization over all decompositions of a state into pure states. For some remarkable cases it happens that such minimizations can be performed analytically [10–13]; however, in the general case these problems are not solved. Therefore, to take a realistic point of view, one can try to estimate entanglement measures, and many proposals for the estimation of entanglement measures have been presented [14–18].

In an experimental setting, the situation becomes even more complicated: since quantum state tomography for multiparticle systems requires an exponentially increasing effort, the state is often not completely known. Typically, one measures so-called entanglement witnesses, special observables, for which a negative expectation value signals the presence of entanglement [19–25]. In this sense, entanglement witnesses allow one to detect entanglement, but the question arises whether they also allow one to quantify entanglement. This question has been addressed from several perspectives [26–30] and in Refs. [31,32] a general recipe for this problem was found. There a method was given for deriving the optimal lower bound on a generic entanglement measure from the expectation value of a witness or another observable. The estimate uses Legendre transforms to give lower bounds on the convex entanglement measure, and the main task in this scheme is to compute the Legendre transform of a given entanglement measure.

In this paper, we extend this method in several directions. First, we derive a simple algorithm for the calculation of the Legendre transform for the concurrence [4] and extensions thereof. Then, we present analytical results for the Legendre

transform for certain witnesses for the geometric measure of entanglement [7]. Finally, we discuss examples and compare our results to other methods for entanglement estimation. But before presenting the new results, let us briefly review the method presented in Refs. [31,32].

### II. THE METHOD

Let us consider the following situation: in an experiment, an entanglement witness  $\mathcal{W}$  has been measured and the mean value  $\langle \mathcal{W} \rangle = \text{Tr}(\varrho \mathcal{W}) = w$  has been found. The task is now to derive from this single expectation value a quantitative statement about the entanglement present in the quantum state. In our case, we aim at providing a lower bound on the entanglement inherent in the state  $\varrho$ . That is, we are looking for statements like

$$\text{Tr}(\varrho \mathcal{W}) = w \Rightarrow E(\varrho) \geq f(w), \quad (1)$$

where  $E(\varrho)$  denotes an arbitrary convex and continuous entanglement measure. We do not specify it further at this point. Naturally, we aim to derive an optimal bound  $f(w)$ , and an estimate is optimal if there is a state  $\varrho_0$  with  $\text{Tr}(\varrho_0 \mathcal{W}) = w$  and  $E(\varrho_0) = f(w)$ .

In order to derive such lower bounds, let us consider the so-called Legendre transform of  $E$  for the witness  $\mathcal{W}$ , defined via the maximization

$$\hat{E}(\mathcal{W}) = \sup_{\varrho} \{ \text{Tr}(\mathcal{W}\varrho) - E(\varrho) \}. \quad (2)$$

As this is defined as the maximum over all  $\varrho$ , we have for any fixed  $\varrho$  that  $\hat{E}(\mathcal{W}) \geq \text{Tr}(\mathcal{W}\varrho) - E(\varrho)$ ; hence

$$E(\varrho) \geq \text{Tr}(\mathcal{W}\varrho) - \hat{E}(\mathcal{W}), \quad (3)$$

which is known as Fenchel's inequality or Young's inequality. The point is that the first term on the right-hand side contains the given measurement data, while the second term can be computed. Therefore, a measurable bound on  $E(\varrho)$  has been obtained.

In order to improve this bound, note that knowing the data  $\text{Tr}(\varrho \mathcal{W}) = w$  is, of course, equivalent to knowing  $\text{Tr}(\varrho \lambda \mathcal{W})$

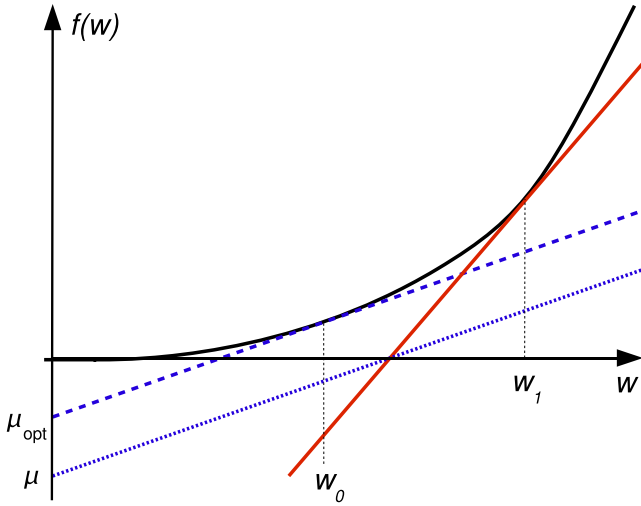


FIG. 1. (Color online) Geometrical interpretation of the Legendre transform. The dotted line is a general affine lower bound, and the dashed line is an optimized bound with the minimal  $\mu$ . By varying the slope, one finds an affine lower bound, which is tight for a given  $w_1$  (solid line). See text for details.

$=\lambda w$  for any  $\lambda$ . Therefore, we can optimize over all  $\lambda$  and obtain

$$E(\varrho) \geq \sup_{\lambda} \{\lambda \text{Tr}(\mathcal{W}\varrho) - \hat{E}(\lambda\mathcal{W})\}. \quad (4)$$

This is a better bound than Eq. (3) and, as we will see, already the optimal bound in Eq. (1).

For our later discussion, it is important to note that this estimation has a clear geometrical meaning (see Fig. 1). As  $E(\varrho)$  is convex, the minimal  $E(\varrho)$  compatible with  $\text{Tr}(\varrho\mathcal{W})=w$ , denoted by  $f(w)$ , is convex, too [33]. Let us consider a generic affine lower bound  $g(w)=\lambda w-\mu$  on  $f(w)$ , i.e.,  $f(w)\geq\lambda w-\mu$ . We have  $\mu\geq\lambda w-f(w)$ , and in order to make the bound for a fixed  $\lambda$  as good as possible, we have to choose  $\mu$  as small as possible. This leads to  $\mu_{\text{opt}}=\sup_w\{\lambda w-f(w)\}$  which is exactly the optimization in Eq. (2).

For a fixed slope  $\lambda$  we obtain by this method an affine bound (characterized by  $\mu_{\text{opt}}$ ) which is already optimal for a certain value  $w_0$ , as it touches  $f(w)$  in this point. For any other mean value  $w$  it delivers a valid, but not necessarily optimal, bound. To obtain the optimal bound for any given  $w_1$  we have to vary the slope  $\lambda$ . This corresponds to the optimization in Eq. (4). Since  $f$  is convex, we obtain for each  $w$  the tight linear bound, showing that this optimization procedure gives indeed the best possible bounds in Eq. (1).

Three remarks are in order at this point. First, it was not necessary for  $\mathcal{W}$  to be an entanglement witness; we may consider an arbitrary observable instead. Second, we can also consider a set of observables  $\vec{\mathcal{W}}=\{\mathcal{W}_1, \dots, \mathcal{W}_n\}$  at the same time. We just have to introduce a vector  $\vec{\lambda}=\{\lambda_1, \dots, \lambda_n\}$  and replace  $\lambda\mathcal{W}$  by  $\sum_k\lambda_k\mathcal{W}_k$ , then all formulas remain valid. Finally, also for a nonconvex  $E(\rho)$  the method delivers valid bounds; however, then it is not guaranteed that the bounds are the optimal ones.

In any case, the method relies vitally on the ability to compute the Legendre transform in Eq. (2). The difficulty of this task clearly depends on the witness  $\mathcal{W}$  and on the measure  $E(\varrho)$  chosen. At first sight, the task may seem hopeless, as the calculation of  $E(\varrho)$  for mixed states is for many measures already impossible.

For instance, a large class of entanglement measures is defined via the convex roof construction. For that, one first defines the measure  $E(|\psi\rangle)$  for pure states, and then defines for mixed states

$$E(\varrho) = \inf_{\sum_k p_k |\phi_k\rangle} \sum_k p_k E(|\phi_k\rangle), \quad (5)$$

where the infimum is taken over all possible decompositions of  $\varrho$ , i.e., over all  $p_k$  and  $|\phi_k\rangle$  with  $\varrho=\sum_k p_k |\phi_k\rangle\langle\phi_k|$ . Clearly, this infimum is very difficult to compute.

However, for the computation of the Legendre transform, this is not relevant: as one can easily prove (see Ref. [31] for details), for convex roof measures the maximization has to run only over pure states,

$$\hat{E}(\mathcal{W}) = \sup_{|\psi\rangle} \{\langle\psi|\mathcal{W}|\psi\rangle - E(|\psi\rangle)\}, \quad (6)$$

which simplifies the calculation significantly. In fact, this shows that for convex roof measures, which are by construction rather difficult to compute, the Legendre transform is rather simple to compute.

In Ref. [31] we considered the entanglement of formation and the geometric measure of entanglement as entanglement measures, which are both convex roof measures. We provided simple algorithms for the calculation of the Legendre transform, and for special witnesses, we calculated the Legendre transform of the geometric measure also analytically. In this paper, we will consider the concurrence and extensions thereof, and we will also present new analytical results for the geometric measure.

Finally, it should be noted that the optimization in Eq. (4) can be completely skipped. Any  $\lambda$  already delivers a valid bound. However, the optimal  $\lambda$  can easily be found numerically.

### III. THE CONCURRENCE

As a first entanglement measure, let us discuss the concurrence. This quantity is defined for pure states as [4]

$$E_C(|\psi\rangle) = \sqrt{2[1 - \text{Tr}(\varrho_A^2)]}, \quad (7)$$

where  $\varrho_A$  the reduced state of  $|\psi\rangle$  for Alice. For mixed states this definition is extended via the convex roof construction in Eq. (5). For the special case of two qubits, the concurrence is a monotonic function of the entanglement of formation, moreover, the minimization in the convex roof construction can be explicitly performed [10]. In the general case, it is not so directly connected to the entanglement of formation. The concurrence is an entanglement monotone [35], but it does not satisfy all desired axioms for an entanglement measure, e.g., it is not additive.

Here, we want to calculate the Legendre transform of  $E_C$  for a generic witness  $\mathcal{W}$ . Similarly to what was done in Ref.

[31] for the entanglement of formation, we will construct an iterative algorithm for the optimization, which converges to the maximum as a fixed point.

First, as the concurrence is defined via the convex roof, it suffices in Eq. (2) to optimize over pure states only. Then, using the fact that for  $x \in [0; 1]$

$$\sqrt{x} = \inf_{\alpha \in [0; 1]} \left\{ \frac{x}{2\alpha} + \frac{\alpha}{2} \right\}, \quad (8)$$

we can rewrite the Legendre transform as

$$\hat{E}_C(\mathcal{W}) = \sup_{|\psi\rangle} \sup_{\alpha} \left\{ \langle \psi | \mathcal{W} | \psi \rangle - \frac{1 - \text{Tr}(\varrho_A^2)}{\sqrt{2}\alpha} - \frac{\alpha}{\sqrt{2}} \right\}. \quad (9)$$

The idea is to write this maximization as an iteration that optimizes  $\alpha$  and  $|\psi\rangle$  in turn. For a fixed  $|\psi\rangle$  we perform the maximization over  $\alpha$  analytically and similarly we can find the optimal  $|\psi\rangle$  for a fixed  $\alpha$ . Concerning the first step, note that for a fixed  $|\psi\rangle$  the optimal  $\alpha$  is simply given by

$$\alpha = \sqrt{1 - \text{Tr}(\varrho_A^2)}. \quad (10)$$

Concerning the second step, if  $\alpha$  is fixed, we have essentially to solve an optimization problem like

$$\sup_{|\psi\rangle} \{ \langle \psi | \tilde{\mathcal{W}} | \psi \rangle - [1 - \text{Tr}(\varrho_A^2)] \}, \quad (11)$$

where  $\tilde{\mathcal{W}}$  is proportional to the original witness  $\mathcal{W}$ .

Here, the second term is nothing but the  $q$  entropy, investigated in detail by Havrda, Charvat, Daróczy, and Tsallis [36–39],

$$S_q(\varrho) = \frac{1 - \text{Tr}(\varrho^q)}{q - 1}, \quad (12)$$

for the case  $q=2$ . Therefore, we can try to write  $S_q(\varrho_A)$  as an infimum via the Gibbs principle, similarly to what was done for the von Neumann entropy in Ref. [31].

So we make the ansatz

$$S_2(\varrho) = \inf_H \{ \text{Tr}(\varrho H) - F_2(H) \}, \quad (13)$$

$$F_2(H) = \inf_{\varrho} \{ \text{Tr}(\varrho H) - S_2(\varrho) \}. \quad (14)$$

For the case of the von Neumann entropy these formulas just express the Gibbs variational principle, where  $F$  is the free energy, and the inverse temperature was set to  $\beta=1$ .

We are mainly interested in the first minimization and have to compute  $F_2$  and the  $H$ , where the minimum is attained. The point is that the second minimization has been solved already by Guerberoff and Raggio [40] and the unique thermal state minimizing Eq. (14) for an arbitrary Hamiltonian  $H$  and consequently  $F_2$  is known. For the first minimization, it remains to find the Hamiltonian for which the given state is the thermal state.

In order to do this in practice, let us first recall the results of Ref. [40]. For the case  $q=2$  and  $\beta>0$ , the results of this reference state the following.

Let  $H$  be a Hamiltonian with ground state energy  $\varepsilon_-$ , ground state degeneracy  $g_-$ , and let the energy of the first excited state be  $\varepsilon_-^*$ . Define

$$\beta^+ = \frac{2}{g_-(\varepsilon_-^* - \varepsilon_-)} > 0 \quad \text{and} \quad t^+ = \frac{1}{(\varepsilon_-^* - \varepsilon_-)} > 0, \quad (15)$$

and the monotonically increasing function  $\beta(t) : [0, t^+] \rightarrow [0, \beta^+]$  as

$$\beta(t) = \frac{2t}{\text{Tr}([1 - t(H - \varepsilon_- \mathbb{1})]_{\oplus})}, \quad (16)$$

where  $[X]_{\oplus}$  denotes the positive part of the operator  $X$ . Let  $\tau$  be the inverse function to  $\beta(t)$ .

Then, for  $\beta < \beta^+$  the unique thermal state is given by

$$\varrho = \mathcal{N}([1 - \tau(\beta)(H - \varepsilon_- \mathbb{1})]_{\oplus}) \quad (17)$$

where  $\mathcal{N}$  denotes the normalization, and for  $\beta \geq \beta^+$  the thermal state is just the normalized projector onto the eigenspace corresponding to the lowest energy  $\varepsilon_-$ . From this, it is clear that  $\varrho$  and  $H$  are diagonal in the same basis.

Coming back to the minimizations in Eqs. (13) and (14) let us assume that a density matrix  $\varrho$  with decreasing eigenvalues  $\lambda_i$  ( $i=1, \dots, N$ ) is given, and the task is to compute the corresponding Hamiltonian  $H$  with increasing eigenvalues  $E_i$ . Without losing generality, we can choose  $E_1=0$ .

Let us first consider the case that  $\varrho$  is nondegenerate and has full rank. Then, Eq. (17) implies that the eigenvalues  $E_i$  of  $H$  have to satisfy  $1 - \tau(\beta)E_i > 0$  for all  $i$ . Since we are considering the case  $\beta=1$ , we have for  $\tau_0 = \tau(\beta=1)$  due to Eq. (16) that  $\tau_0 = [\text{Tr}(1 - \tau_0 H)]/2$ . From Eq. (17) it follows first that  $\lambda_1 = \mathcal{N} = 1/\text{Tr}(1 - \tau_0 H) = 1/(2\tau_0)$ , and then  $\lambda_i = \lambda_1(1 - \tau_0 E_i) = \lambda_1[1 - E_i/(2\lambda_1)]$ ; hence

$$E_i = 2(\lambda_1 - \lambda_i). \quad (18)$$

For this Hamiltonian, we have also

$$F_2(H) = 2\lambda_1 - \sum_i \lambda_i^2 - 1. \quad (19)$$

As a remark, first note that this solution satisfies  $1 - \tau(\beta)E_i = 1 - (\lambda_1 - \lambda_i)/\lambda_1 > 0$ , as requested at the beginning. Second, it delivers  $\beta^+ = 1/(\lambda_1 - \lambda_2) > \beta=1$ , justifying the ansatz in Eq. (17). Finally, it is easy to see that if  $\varrho$  is not of full rank or is degenerate, the recipe above works also and delivers a correct solution.

In summary, we can write the problem of the computation of the Legendre transform for the concurrence as

$$\hat{E}_C(\mathcal{W}) = \sup_{|\psi\rangle} \sup_H \sup_{\alpha} \left\{ \langle \psi | \mathcal{W} | \psi \rangle - \frac{1}{\sqrt{2}\alpha} [\langle \psi | (H \otimes \mathbb{1}) | \psi \rangle - F_2(H)] - \frac{\alpha}{\sqrt{2}} \right\}. \quad (20)$$

If  $|\psi\rangle$  and  $H$  are fixed, we can compute the optimal  $\alpha$  as shown at the beginning. If  $|\psi\rangle$  and  $\alpha$  are fixed, we can determine the optimal  $H$  as above. Finally, if  $H$  and  $\alpha$  are fixed we choose  $|\psi\rangle$  as the eigenvector corresponding to the maximal eigenvalue of  $\mathcal{W} - (H \otimes \mathbb{1})/(\sqrt{2}\alpha)$ . Therefore, we have an it-

erative optimization, which delivers a monotonically increasing sequence of values for the Legendre transform, with the actual value as a fixed point.

This algorithm can be implemented with a few lines of code; examples will be discussed in Sec. V. It should be noted that in principle we cannot prove that the algorithm converges always to the global optimum, as the final fixed point may depend on the starting values of  $|\psi\rangle$ ,  $H$ , and  $\alpha$ , leading to an overestimation of the concurrence. In practice, however, the convergence behavior is quite well behaved, and the algorithm delivers a well-suited tool for obtaining sharp bounds on the concurrence.

Finally, let us add that with the same method also extensions of the concurrence may be treated. For instance, one may consider quantities for pure states as  $E_q(|\psi\rangle) = S_q(\varrho_A)$ . With the convex roof extension, these are also entanglement monotones [35], and, using the results of Ref. [40], the Legendre transform can be calculated in a similar manner as above.

In addition, there are several multipartite entanglement monotones, which can be seen as multipartite extensions of the concurrence [5,9,41]. For instance, for  $N$ -qubit states one can define the Meyer-Wallach measure

$$E_{\text{MW}}(|\psi\rangle) = 2 \left( 1 - \frac{1}{N} \sum_{k=1}^N \text{Tr}(\varrho_k^2) \right), \quad (21)$$

where the  $\varrho_k$  are all reduced one-qubit states. Clearly, due to the similar structure as in Eq. (7) the methods from above can also be used to compute the Legendre transformation for these measures.

#### IV. THE GEOMETRIC MEASURE

As the second entanglement measure, let us consider the geometric measure of entanglement  $E_G$  [7]. This is an entanglement monotone multipartite system, quantifying the distance to the separable states. The geometric measure is defined for pure states as

$$E_G(|\psi\rangle) = 1 - \sup_{|\phi\rangle=|a\rangle|b\rangle|c\rangle\cdots} |\langle\phi|\psi\rangle|^2, \quad (22)$$

i.e., as one minus the maximal overlap with pure fully separable states, and for mixed states via the convex roof construction.

The geometric measure is a *multipartite* entanglement measure, as it is not only a summation over bipartite entanglement properties. Despite its abstract definition, it has turned out that  $E_G$  can be used to quantify the distinguishability of multipartite states by local means [43]. As the geometric measure is one of the few measures for multipartite systems that has a reasonable operational meaning and at the same time is proved to satisfy all of the conditions for entanglement monotones, it has been investigated from several perspectives, for instance it has been used to study multipartite entanglement in condensed matter systems [44].

In Ref. [31] the problem of calculating the Legendre transform for the geometric measure was already considered and the following results were obtained. First, an iterative

algorithm (in the same spirit as the algorithm for the concurrence in the previous section) was derived for calculating the Legendre transform of arbitrary witnesses. Second, for the important case that the witness is of the form  $\mathcal{W} = \alpha \mathbb{1} - |\chi\rangle\langle\chi|$  (or, equivalently,  $\mathcal{W} = |\chi\rangle\langle\chi|$ ) an analytic formula of the Legendre transform has been derived, reading,

$$\hat{E}_G(r\mathcal{W}) = \begin{cases} r\alpha & \text{for } r \geq 0, \\ \left[ \sqrt{(1-r)^2 + 4rE_G(|\chi\rangle)} + 2\alpha r - r - 1 \right] / 2 & \text{for } r < 0. \end{cases} \quad (23)$$

Here, we want to generalize this result by determining  $\hat{E}_G(\mathcal{W})$  analytically for the case that  $\mathcal{W}$  is diagonal in some special basis, e.g. the Greenberger-Horne-Zeilinger (GHZ) state basis. We first consider the special case of the GHZ state basis, then the formula for the general case can directly be written down.

So let us assume that

$$\mathcal{W} = \sum_{i=1}^{2^N} \lambda_i |\text{GHZ}_i\rangle\langle\text{GHZ}_i| \quad (24)$$

is the witness for an  $N$ -qubit system, where  $|\text{GHZ}_i\rangle = (|x^{(1)}\cdots x^{(N)} \pm |y^{(1)}\cdots y^{(N)}\rangle) / \sqrt{2}$  with  $x^{(i)}, y^{(i)} \in \{0, 1\}$  and  $x^{(i)} \neq y^{(i)}$  is the GHZ state basis. Without losing generality we assume that the  $\lambda_i$  are decreasingly ordered, i.e.,  $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{2^N}$ , but not necessarily positive.

The Legendre transform is given by

$$\begin{aligned} \hat{E}_G(\mathcal{W}) &= \sup_{|\psi\rangle} \sup_{|\phi\rangle=|a\rangle|b\rangle|c\rangle\cdots} \langle\psi|[\mathcal{W} + |\phi\rangle\langle\phi|]|\psi\rangle - 1 \\ &= \sup_{|\phi\rangle=|a\rangle|b\rangle|c\rangle\cdots} \|[\mathcal{W} + |\phi\rangle\langle\phi|]\| - 1, \end{aligned} \quad (25)$$

where  $\|X\|$  denotes the maximal eigenvalue of the operator  $X$ . In order to compute this maximal eigenvalue, we write the operator  $[\mathcal{W} + |\phi\rangle\langle\phi|]$  in the GHZ basis.  $\mathcal{W}$  is diagonal there and since the maximal overlap between the fully separable state  $|\phi\rangle$  and any of the GHZ states is  $1/2$  (i.e., the geometric measure for GHZ states is  $1/2$  [7]), the matrix representation of  $|\phi\rangle\langle\phi|$  has matrix elements with absolute values not larger than  $1/2$ .

Our claim is now that the optimal choice of  $|\phi\rangle$  is to take  $|\phi\rangle\langle\phi|$  as a  $2 \times 2$  matrix with all entries  $1/2$  and acting on the two-dimensional space corresponding to the largest eigenvalues  $\lambda_1$  and  $\lambda_2$ . To prove that this choice is really optimal, we show that the above mentioned choice is also optimal if we consider the more general class of all  $|\phi\rangle$ , which have an overlap smaller than or equal to  $1/2$  with all the GHZ states, but which are not necessarily product states.

We prove it by contradiction. Let us assume a different optimal solution  $|\phi\rangle$  and a corresponding eigenvector to the maximal eigenvalue  $|\psi\rangle$ . The vectors can be written as  $|\phi\rangle = \sum_k \alpha_k |\text{GHZ}_k\rangle$  and  $|\psi\rangle = \sum_k \beta_k |\text{GHZ}_k\rangle$ . We assume without losing generality that  $0 < |\alpha_1|^2 < 1/2$  and  $0 < |\alpha_3|^2 < 1/2$ . The function to maximize is given by



$$\hat{E}_G(\mathcal{W}) = \left| \sum_k \alpha_k^* \beta_k \right|^2 + \sum_k |\beta_k|^2 \lambda_k - 1. \quad (26)$$

Since we are interested in the maximum, we can, without restricting generality, assume that  $\alpha_k$  and  $\beta_k$  are real and positive. The interesting terms for the discussion are

$$X = \alpha_1 \beta_1 + \alpha_3 \beta_3, \quad Y = \beta_1^2 \lambda_1 + \beta_3^2 \lambda_3. \quad (27)$$

$X$  is a scalar product, which is maximal if the vectors  $(\alpha_1, \alpha_3)$  and  $(\beta_1, \beta_3)$  are parallel. For given values of  $(\beta_1, \beta_3)$  this may be prohibited by the constraint  $\alpha_i^2 \leq 1/2$ . Then, however, it is clearly optimal to take an  $(\alpha_1, \alpha_3)$  at the border of the domain, which has for one  $\alpha_i = 1/2$ , leading to a contradiction with the assumption on the form of  $|\phi\rangle$ . Otherwise, we can choose the two vectors parallel, and  $(\alpha_1, \alpha_3)$  is not at the border. Then, however, we can enlarge  $Y$  by increasing  $\beta_1$  in  $(\beta_1, \beta_3)$  [and, simultaneously  $\alpha_1$  in  $(\alpha_1, \alpha_3)$  in order to keep the vectors parallel]. This leads to another contradiction concerning the optimality of  $|\psi\rangle$ .

Note that the class of the considered  $|\phi\rangle$  is strictly larger than the class of product vectors, since not for every pair of GHZ states  $|\text{GHZ}_1\rangle$  and  $|\text{GHZ}_2\rangle$  can we find a product vector  $|\phi\rangle$ , such that  $|\phi\rangle$  has an overlap of  $1/2$  with both of the  $|\text{GHZ}_i\rangle$ . However, we obtain an upper bound on the Legendre transform from this ansatz, which can be used for a valid lower bound on the entanglement measure. Further, one can check whether this bound is tight by direct inspection of  $|\text{GHZ}_1\rangle$  and  $|\text{GHZ}_2\rangle$  afterward.

Having shown that the simplest choice of  $|\phi\rangle$  is optimal, the calculation of the Legendre transform reduces to a calculation of eigenvalues of a  $2 \times 2$  matrix, and we have

$$\begin{aligned} \hat{E}_G(\mathcal{W}) &\leq \left\| \begin{bmatrix} \lambda_1 + 1/2 & 1/2 \\ 1/2 & \lambda_2 + 1/2 \end{bmatrix} \right\| - 1 \\ &= \frac{\lambda_1 + \lambda_2 - 1}{2} + \frac{1}{2} \sqrt{(\lambda_1 - \lambda_2)^2 - 1}. \end{aligned} \quad (28)$$

The generalization to other states besides GHZ states is straightforward: if the overlap is bounded by some other number (e.g.,  $1/4$  for four-qubit cluster states), we only have to calculate the eigenvalues of some larger matrix (e.g., a  $4 \times 4$  matrix for four-qubit cluster states), in order to derive an analytical upper bound on  $\hat{E}_G(\mathcal{W})$ . We can summarize as follows.

*Observation.* Let  $\mathcal{W} = \sum_{i=1}^{2^N} \lambda_i |\psi_i\rangle\langle\psi_i|$  be an operator, where for all eigenvectors  $|\psi_i\rangle$  the overlap with fully separable states is bounded by  $1/k, k \in \mathbb{N}$ . Then the Legendre transform is bounded by

$$\hat{E}_G(\mathcal{W}) \leq \|[X]\| - 1 \quad (29)$$

where  $X$  is a  $k \times k$  matrix with the entries  $\lambda_i + 1/k$  on the diagonal, and off-diagonal entries  $1/k$ . The question whether this bound is the exact value can be decided by direct inspection of the  $|\psi_i\rangle$ .

This observation allows for a simple calculation of a lower bound on  $E_G$  if the fidelities of the basis states  $|\psi_i\rangle$  are known. First, the estimation is much simpler and faster compared with the iteration algorithm for arbitrary witnesses,

since the optimization runs only over the  $k$  largest eigenvalues  $\lambda_i$  of the possible witnesses  $\mathcal{W} = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$ . For the iteration algorithm, it would be necessary to consider all witnesses  $\mathcal{W} = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$ , which amounts to a variation over  $2^N$  parameters  $\lambda_i$ . Second, the bounds on  $E_G$  may become significantly better, compared with the estimation from a single fidelity, according to Eq. (23).

For example, the  $|\psi_i\rangle$  may be a graph state basis, where the fidelities have been determined from the expectation values of the stabilizer operators [23]. In Sec. V we will discuss an example for four-qubit states.

## V. EXAMPLES

In this section, we present several examples for the presented method and compare it with other estimation methods as well as with exact values of the entanglement measures. A MATHEMATICA file with the algorithms used for the calculation of the Legendre transforms is available from the authors.

### A. Concurrence for isotropic states

As a first example, let us consider isotropic states in an  $N \times N$  system, defined by

$$\varrho(F) = \frac{1-F}{N^2-1} (1 - |\phi\rangle\langle\phi|) + F |\phi\rangle\langle\phi|, \quad (30)$$

which is a convex combination of a maximally entangled state  $|\phi\rangle = \sum_i |ii\rangle / \sqrt{N}$  and the totally mixed state. The parameter  $F$  encodes the fidelity of  $|\phi\rangle$ , i.e.,  $F = \langle\phi| \varrho(F) |\phi\rangle$ . For these states, the concurrence is known to be [12]

$$C(\varrho) = \sqrt{\frac{2N}{N-1} \left( F - \frac{1}{N} \right)}. \quad (31)$$

In order to test our methods, we consider the standard witness for states of the form in Eq. (30), namely,

$$\mathcal{W} = \frac{1}{N} - |\phi\rangle\langle\phi|, \quad (32)$$

and estimate from its expectation value the concurrence, using our algorithm. The results for the case  $N=3$  are shown in Fig. 2. It turns out that, for this case, our lower bounds are sharp and reproduce the exact value of the concurrence.

### B. Comparison with other estimation methods

Let us compare the presented estimation method with other methods of estimating entanglement measures. With this aim, we consider two-qubit states of the form

$$\varrho(p) = p |\psi\rangle\langle\psi| + (1-p) \sigma, \quad (33)$$

where  $|\psi\rangle$  is a pure entangled state and  $\sigma$  is unknown and random separable noise. As entanglement measure we consider the entanglement of formation. This is, for the case of two qubits, equivalent to the concurrence, since it is a monotonic function of it. We consider six different methods for estimating the entanglement of formation.

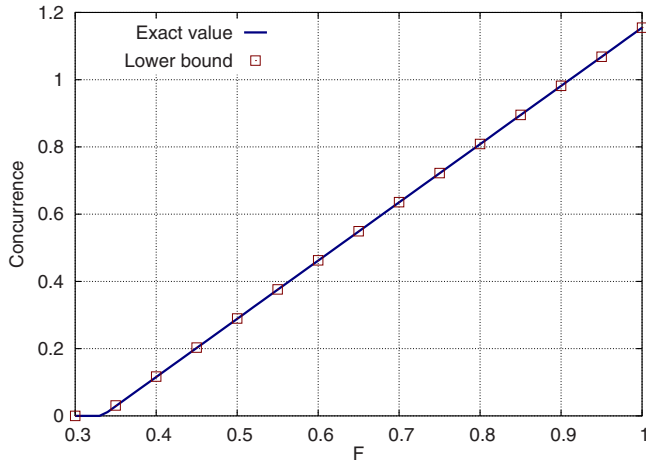


FIG. 2. (Color online) Exact value of the concurrence and a lower bound from the witness in Eq. (32) and the algorithm in Sec. IV for isotropic states. See text for details.

(1) For the two-qubit case we can exactly calculate the entanglement of formation using the formula of Wootters [10]. Clearly, since this requires complete knowledge of the density matrix, for an experimental implementation state tomography is needed.

(2) In Refs. [14,15] a method to estimate the entanglement of formation or the concurrence from the separability criterion of the positivity of the partial transpose or the computable cross norm or realignment criterion was presented. Experimentally, this approach again requires state tomography.

(3) We can also take the witness that is proper for states of the form  $\varrho(p) = p|\psi\rangle\langle\psi| + (1-p)\mathbb{1}/4$ . This witness might not be the optimal one for the state under investigation, since the noise is not known and is in general white. However, we can use the Legendre transform with the algorithm of Ref. [31] to estimate the entanglement of formation from it. Equivalently, we can use the algorithm of Sec. III to estimate the concurrence. Experimentally, this method does not require state tomography; only three local measurements are needed for the measurement of the witness [45].

(4) The witness in the third method is of the form

$$\mathcal{W} = |\phi\rangle\langle\phi|^{T_B}. \quad (34)$$

Clearly, the mean value  $\langle\mathcal{W}\rangle = \text{Tr}(\varrho_{\text{expt}}\mathcal{W}) = \langle\phi|\varrho_{\text{expt}}^{T_B}|\phi\rangle$  can be used to derive a lower bound on the negativity of the partial transpose  $\varrho_{\text{expt}}^{T_B}$ . Then, the second method [14,15] may be used to estimate the entanglement of formation. This approach does not require state tomography.

(5) In Ref. [16] lower bounds on the concurrence from measurements on two copies of the state  $\varrho$  were derived. For the case of two qubits we can use them to bound also the entanglement of formation. A measurement of a single observable on two copies can always be expressed as a function of mean values of local observables on a single copy. In this case, however, for such an implementation to be effective, state tomography is needed.

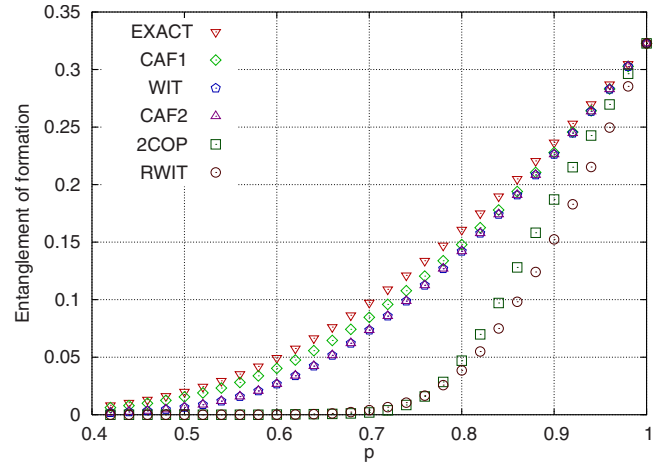


FIG. 3. (Color online) Comparison of different methods to estimate the entanglement of formation for noisy two-qubit states. EXACT denotes the exact calculation according to Ref. [10]; CAF1 the second method, estimating the entanglement from the PPT criterion, from Chen, Alberverio, and Fei [14,15]; WIT the estimation from the witness as presented in this paper and in Ref. [31]; CAF2 the fourth method as a combination of the witness with CAF1; 2COP the fifth method, using measurements on two copies [16]; and RWIT the sixth method [30]. See text for details.

(6) In Ref. [30] a method for estimating the concurrence from special entanglement witnesses has been derived. That is, it was shown that

$$E_C(\varrho) \geq -\frac{1}{E_C(|\phi\rangle)}\langle\mathcal{W}_\phi\rangle, \quad (35)$$

where  $\mathcal{W}_\phi = 2[\mathbb{1}_A \otimes \text{Tr}_A(|\phi\rangle\langle\phi|) - |\phi\rangle\langle\phi|]$  is a witness belonging to the reduction criterion. We use this method with the witness  $W_\psi$  for the state  $|\psi\rangle$ . With this choice, the method automatically reproduces the exact value for the case  $p=1$  and it can be seen that Eq. (35) is nothing but the Legendre transform for a special choice of the slope  $\lambda$ . Experimentally, this method would also require three local measurements [30,45].

As an example, we considered in Eq. (33) the pure state  $|\psi\rangle = (4|00\rangle + |11\rangle)/\sqrt{17}$  and the state  $\sigma$  was randomly (in the Hilbert-Schmidt measure) chosen from the set of separable states [46]. For a fixed  $\sigma$  we calculated all the above mentioned values depending on the noise level  $p$  and finally averaged over hundred realizations of  $\sigma$ . The results are shown in Fig. 3 and Table I.

One can clearly see that the methods 2, 3, and 4 result in bounds on the entanglement of formation that are very close to the exact result. The second method is the best bound; however, it requires complete knowledge of the state. The third method is by construction better than the fourth method (as the Legendre transform delivers by construction the best possible bounds from a given witness). In this example, however, they are practically equivalent. The fifth and sixth methods deliver good results if  $\varrho$  is close to a pure state.

TABLE I. Comparison of the different estimation methods. For each method, the required number of local measurement settings on a single copy and the efficiency  $\eta$  are given. Here, the efficiency is defined as the ratio between the estimated value of the entanglement of formation and the actual one, for two different regions of the noise parameter  $p$ .

Method	CAF1	WIT	CAF2	2COP	RWIT
No. of measurements	9	3	3	9	3
$\eta$ for $p \in [0.8; 1.0]$	96.0%	94.8%	94.8%	70.1%	63.0%
$\eta$ for $p \in [0.6; 0.8]$	86.0%	72.0%	72.0%	5.9%	7.0%

C. Geometric measure for four-qubit states

As a third example we discuss the geometric measure of entanglement. In order to demonstrate the method in Sec. IV, we consider an experimental situation similar to the one in Ref. [23]. In this experiment, a four-photon cluster state

$$|CL\rangle = \frac{1}{2}(|0000\rangle + |0011\rangle + |1100\rangle - |1111\rangle) \quad (36)$$

has been prepared using parametric down-conversion and a controlled phase gate. The fidelity of the target state was then determined by the measurement of all stabilizer operators. These operators are given by the local observables  $S_1 = \sigma_z \sigma_z \mathbb{1} \mathbb{1}$ ,  $S_2 = \sigma_x \sigma_x \sigma_z \mathbb{1}$ ,  $S_3 = \mathbb{1} \sigma_z \sigma_x \sigma_x$ , and  $S_4 = \mathbb{1} \mathbb{1} \sigma_z \sigma_z$ , and products of these observables. The cluster state is an eigenstate (with eigenvalue +1) of all these  $2^4=16$  observables, and from their expectation values the fidelity can be determined [21,23].

Using the fact that the maximal overlap of the cluster state with fully separable states equals 1/4 (i.e., the geometric measure is 3/4 [42]) Eq. (23) can be used to bound  $E_G$  from this fidelity. There are, however, also other common eigenstates of the  $S_i$  with different eigenvalues. These states are orthogonal to the cluster state and form the so-called cluster state basis. All states in this basis share the same entanglement properties and their fidelities can also be determined from the mean values of the  $S_i$ . In fact, the knowledge of all  $\langle S_i \rangle$  is equivalent to the knowledge of all fidelities.

In order to investigate how the information about the fidelities of all states in the cluster state basis can be used for the estimation of entanglement, we consider the simple case that only three fidelities are larger than zero,  $F_1$ ,  $F_2$ , and  $F_3=1-F_1-F_2$ . For a given triple of fidelities we may first consider the maximal fidelity and then use Eq. (23) to obtain a lower bound on  $E_G$ . Alternatively, we can use the methods of Sec. IV and consider all three fidelities at the same time. In practice, this gives a lower bound on  $E_G$  by the optimization problem

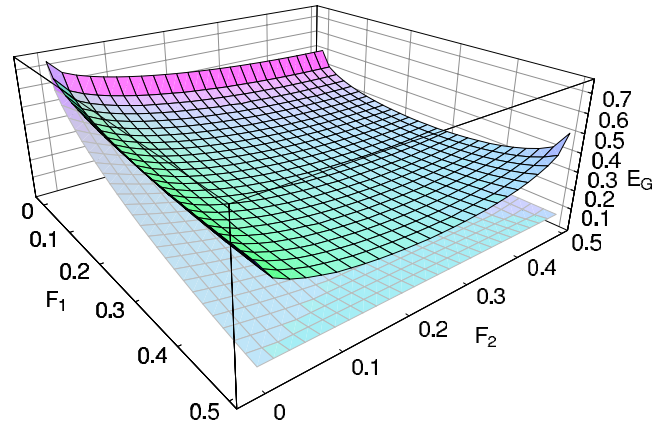


FIG. 4. (Color online) Comparison between two estimation methods for the geometric measure of entanglement. The lower curve is the analytical bound from the maximal fidelity according to Ref. [31] or Eq. (23), the upper curve is the analytical bound from Sec. IV, taking all fidelities into account. See text for details.

$$E_G \geq \sup_{\lambda_1, \dots, \lambda_4} \left\{ \sum_{k=1}^3 \lambda_k F_k - \|[X]\| + 1 \right\}, \quad (37)$$

where  $X$  is defined as in Eq. (29) for  $k=4$ . Any set of  $\lambda_i$  delivers already a valid lower bound, and the optimum over all  $\lambda_i$  is easily found.

The results are plotted in Fig. 4. One can clearly see that taking all fidelities into account improves the lower bounds significantly.

VI. CONCLUSION

In conclusion, we have investigated how entanglement measures can be estimated from incomplete experimental data. We have shown that the method of Legendre transforms can successfully be applied to the concurrence and extensions thereof. Furthermore, we have presented an analytical way to estimate the geometric measure if the fidelities of certain basis states are known. Extending the presented methods to other entanglement measures is an interesting task for further study.

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